

Current induced spin flip scattering at interfaces in noncollinear magnetic multilayers

Peter M Levy and Jianwei Zhang

Department of Physics, 4 Washington Place, New York University, New York, New York 10003

(Date: February 6, 2008; Received textdate)

We show that when one drives a charge current across noncollinear magnetic layers the two electron Coulomb scattering creates a spin flip potential at interfaces. This scattering is found when the interface potential is updated due to the spin accumulation attendant to charge flow, and it contributes in linear response to the current. With this scattering there is an injection of transverse spin distributions in a layer that propagate, and that in the steady state lead to spin currents transverse to the magnetization.

PACS numbers: 72.25.-b, 72.15.Gd, 73.23.-b

Keywords: spin currents, noncollinear structures, Coulomb interaction

Our current knowledge of the electronic structure of magnetic multilayers is based on effective single electron approximations. In nonmagnetic (normal) layers states are spin degenerate while in the magnetic they are spin split; therefore one can construct a coherent combination of spin up and down states in the normal layers, while in the magnetic this is not possible because there is no coherence (correlations) between states in spin split bands.¹ This loss of spin coherence as one crosses a normal/ferromagnetic layer (N/F) interface has been identified as the origin for the inability of injecting transverse spin currents from a normal metal into a 3d transition-metal ferromagnet.² The studies to date of the coherence transmitted by interface scattering have concluded that spin currents across this interface can induce only a transverse coherence between electrons on different sheets of the spin split Fermi surface of the ferromagnet.² Here we revisit this question and find a current driven correction to the transmission amplitudes coming from the two electron Coulomb interaction at interfaces that allows the transverse spin coherence to be carried by the electron distribution function for each spin split band. As we show while this is an out of equilibrium effect, its inclusion in transport calculations enters in linear response. In another publication we show that this current induced coherence make it possible for spin currents to be continuous across the interface in the *steady state*.³ Inasmuch as one includes current driven accumulations in the bulk of the layers when calculating the steady state currents we conclude that to discuss spin currents in noncollinear magnetic structures it is necessary to self consistently update the transmission and reflection coefficients due to the presence of out of equilibrium spin distributions at interfaces.

To relate distribution functions $f_{ss'}(k, r)$ across an interface one resorts to the transfer matrix⁴

$$f_{ss'}^>(k, 0^+) = \sum_{mm'k'} T_{mm' ss'} f_{mm'}^>(\hat{k}', \varepsilon_k, 0^-) + \sum_{mm'k''} R_{mm' ss'} f_{mm'}^<(\hat{k}'', \varepsilon_k, 0^+), \quad (1)$$

where the transmission and reflection coefficients (prob-

abilities) are

$$T_{mm' \Rightarrow ss'} = T_{mm' ss'} = t_{ms} * t_{m's'}^*, \quad (2)$$

$$R_{mm' \Rightarrow ss'} = R_{mm' ss'} = r_{ms} * r_{m's'}^*,$$

and $t_{ms}(k', k, \varepsilon_k), r_{ms}(k'', k, \varepsilon_k)$ are the transmission and reflection amplitudes for elastic scattering. At the interface between a normal and ferromagnetic layer the momenta k, k', k'' are either k_M or k_m , for a majority and minority bands of the ferromagnetic layer and k_n for a normal metal layer. We make the "isotropy" assumption that allows one to write one coefficient for all momentum directions, albeit one should still keep a band index, i.e., $T_{mm' \Rightarrow ss'}(k', k, \varepsilon_k) \sim T_{mm' \Rightarrow ss'}(\varepsilon_k)$.⁴ In a spin polarized single electron description the spin split bands of the magnetic layer have only one spin index, $s = s'$, for each momentum k , i.e., $f_{ss'} = f_s$, however when one is propagating currents across noncollinear structures one has to envisage the possibility of off diagonal components of the distribution function $f_{ss'}^>(k, 0^+)$ with $s \neq s'$ within a screening length about the interface. This represents a coherence between states in different bands; it does not represent an admixture of spin within the band although the scattering we find is capable of this.⁵ The indices m, m' refer to the spin of the electron in the unsplit Fermi sea of the normal metal layer; in nonmagnetic layers it is possible to construct coherent combinations of up and down spin states $m \neq m'$. Scattering at interfaces in metallic structures is localized within a screening length about the interface and represented by amplitudes $t_{m_l \rightarrow m_r}, r_{m_l \rightarrow m_r'}$; the first describe the transmission from, say, the left layer to the right, the second the reflection back into the left layer, and the $m's$ are the components of the electron's spin.

The scattering potential, t matrix, for conduction electrons at an interface between two metals has contributions from differences in, the periodic background potentials, the kinetic energy and the Coulomb interaction between the electrons; when written as an effective one electron potential only the latter changes due to current driven spin accumulation on the Fermi surface. To find these corrections we focus on the electron-electron contribution to the t matrix. The one electron scattering

amplitudes at interfaces are derived from the two electron Coulomb interaction

$$V_{coulomb} = \frac{1}{2} \sum_{\substack{k_1 \dots k_4 \\ s, s'}} V(k_1 s k_2 s' k_3 s' k_4 s) c_{k_1 s}^\dagger c_{k_2 s'}^\dagger c_{k_3 s'} c_{k_4 s}, \quad (3)$$

where $V(k_1 s \dots k_4 s)$ are the matrix elements of the Coulomb interaction between states on either side of the interface. For our purposes the range of integration is limited to the screening length about the interface. As we are working at the interface between dissimilar well screened metals the translational invariance of the background is broken; therefore we do not reduce the four to three momenta. To determine the one electron scattering amplitude, $t_{m_l \rightarrow m_r, r_{m_l} \rightarrow m'_l}$, that arises from this Coulomb interaction we write the Coulomb interaction between electrons in the one electron states in the bulk of the layers on either side of the interface, and to reduce it to a one electron operator we take the expectation value over a pair of annihilation and creation operators in Eq.(3). In the lowest order distorted wave Born approximation the spin dependent part of the correction to the transition matrix between one electron states on the two sides of the interface is⁶

$$t_{m \rightarrow s} = \langle k_2, s | t_{op} | k_n, m \rangle, \quad (4)$$

where

$$t_{op} \equiv -\frac{1}{2} g(\varepsilon_{k_2}) \sum_{k_1 k_3} \left\langle c_{k_1 m}^\dagger c_{k_3 s} \right\rangle V(k_1 m k_2 s k_3 n m) c_{k_2 s}^\dagger c_{k_n m}, \quad (5)$$

$|k_n, m\rangle$ refers to states on the Fermi surface of the normal layer, and $\langle k_2, s|$ to those on the ferromagnetic spin split Fermi surface, so that $k_2 = k_M$ and k_m . For elastic scattering $\delta(\varepsilon_{k_n} - \varepsilon_{k_2})$ the density of states $g(\varepsilon_{k_2})$ enters when one averages the amplitude $t_{m \rightarrow s}$ over the energy ε_{k_n} . While the states in the ferromagnetic layers are pure spin states, e.g., only an up spin goes in the majority sheet, we are looking for current induced coherences in the distribution function, a statistical density matrix, between states of opposite spin; therefore we do not immediately associate a spin s to a state k_2 , e.g., we will be looking for matrix elements for both spin directions on each sheet of the Fermi surface of the ferromagnetic layer that are induced when the system is out of equilibrium.

The expectation value $\langle c_{k_1 m}^\dagger c_{k_3 s} \rangle$ is between states on opposite sides of the interface and is found by self consistently evaluating it there; as we will be interested only in elastic scattering the energy of the states entering this expectation value are the same, $\varepsilon_{k_1} = \varepsilon_{k_3}$, but their directions in k space can be different. At the interface between normal and ferromagnetic layers (N/F) the scattering potential, while spin dependent, is diagonal in spin space, i.e., there is a unique spin direction, and there are no elements $m \neq s$ when the system is in *equilibrium*, and $\langle c_{k_1 m}^\dagger c_{k_3 s} \rangle \sim n_s^{int} \delta_{sm}$; it also follows that $t_{ms}^{eq} = t_s \delta_{sm}$.

When driving current across a magnetic multilayer spin accumulates on the Fermi surface of the normal layers so as to support a spin current across them in steady state, therefore in the presence of a spin current the spin polarized distribution, δn_s^l , of the Fermi surface of the magnetic layer \hat{M}_l upstream from the N/F_r interface is superimposed on the Fermi surface of the normal layer.

For *noncollinear* magnetic layers the magnitude of the current driven accumulation *in the interfacial region* N/F_r coming from the left magnetic layer, δn_s^{int} , is uncertain; this can only be ascertained by a calculation of the transmission amplitudes at N/F_r when one superimposes δn_s^l on the Fermi surface (at the Fermi energy) of the normal layer.⁷ In linear response we do know it is quantized along the magnetization \hat{M}_l of the magnetic layer upstream while the operators entering the expectation value in the interfacial region (see Eq.(5)) are quantized along \hat{M}_r the magnetization of the ferromagnet at the N/F_r interface. To determine the additional contribution from δn_s^l to the transmission amplitude, Eq.(5), it is necessary to rotate the accumulation referred to \hat{M}_l to states quantized along \hat{M}_r ; we find

$$\delta t_{op} \equiv A_{ms}(k_2, k_n) c_{k_2 s}^\dagger c_{k_n m}, \quad (6)$$

where

$$A_{ms}(k_2, k_n) = V_s(k_s k_n; \varepsilon_{k_2}) \times \left\{ \begin{aligned} & [\delta n_s^{int} \cos^2 \theta / 2 + \delta n_s^{int} \sin^2 \theta / 2] \delta_{sm} \\ & - \frac{i}{2} [\delta n_s^{int} - \delta n_{-s}^{int}] \sin \theta \delta_{s, -m} \end{aligned} \right\}, \quad (7)$$

$$V_s(k_2, k_n; \varepsilon_{k_2}) = -\frac{1}{2} g_s(\varepsilon_{k_2}) \langle \langle V(k_2 s, k_{nm}; \varepsilon_F) \rangle \rangle, \quad (8)$$

$$\langle \langle V_s(k_2 s, k_{nm}; \varepsilon) \rangle \rangle = \frac{1}{(4\pi)^2} \int_{\varepsilon_{k_1} = \varepsilon_{k_3} = \varepsilon} d\Omega_{k_1} \int_{\varepsilon_{k_3}} d\Omega_{k_3} V_s(\hat{k}_1, k_2 s, \hat{k}_3, k_{nm}), \quad (9)$$

Here δn_s^{int} is the occupancy of the spin states on the Fermi surface at the interface which have been polarized by the upstream magnetic layer \hat{M}_l .

The out of equilibrium accumulation and current transmitted across an interface N/F by the equilibrium T matrix is found from Eq. (1) by integrating over all k states. For the diagonal spin components $f_{ss'}^> = f_s^> \delta_{ss'}$ the out of equilibrium distribution only exists on the Fermi surface, because $f_{mm'}^>(k', \varepsilon_k, 0^-) \sim \delta f_m(\hat{k}') \delta_{mm'} \delta(\varepsilon_k - \varepsilon_F)$. For spin transport across *noncollinear* magnetic layers the state $|k_n, m\rangle$ is quantized along the magnetization \hat{M}_l of the magnetic layer upstream while the operators in the t matrix are quantized along \hat{M}_r the magnetization of the ferromagnet at the N/F interface, i.e., $\theta = \cos^{-1}(\hat{M}_l \cdot \hat{M}_r)$, therefore it is necessary write $|k_n, m\rangle$ in terms of $|k_2, s\rangle$. By rotating this state we find the average of the transmission coefficient in equilibrium is

$$T_{mm \Rightarrow ss}(\varepsilon_F) = |t_s|^2 \{ \cos^2 \theta / 2 \delta_{sm} + \sin^2 \theta / 2 \delta_{s, -m} \}, \quad (10)$$

where $t_s = t_{ms}^{eq} \delta_{sm}$. As the spin diagonal term $\sim \delta_{sm}$ in Eq.(7) is proportional to the accumulation or current it does not enter in linear response in the T matrix that connects the spin diagonal part of out of equilibrium distribution functions, $f_s^>$ and $\delta f_m(\hat{k}')$, as they themselves produce the accumulation and current when integrated over the Fermi surface. However the off diagonal (spin flip) term $\sim \delta_{s-m}$ in Eq.(7) is uncompensated because the accumulation coming from the right layer at the N/F_r is diagonal in spin space, and cannot offset an off diagonal term coming from the left. At the other interface of the normal layer, N/F_l, the accumulation arising from the right layer δn_s^r cannot be fully compensated from that arising from the left layer and we have an uncompensated contribution $\delta t_{op} \sim \delta_{s,-m}$.⁸

The current driven coherences $f_{ss'}^>$ with $s \neq s'$ do not represent populations, that in equilibrium are given by the Fermi Dirac distribution function, therefore their contribution to the transmission across an interface is *not* limited to the Fermi surface ($\varepsilon_k \neq \varepsilon_F$) and has contributions from the entire Fermi sea. As the scattering potential, Eq.(6), is proportional to the accumulation or current its contribution in linear response to the spin coherence transmitted across an interface is found by using the equilibrium distribution in the normal layer $f^0(\varepsilon_k, 0^-) \delta_{mm'}$ in Eq.(1), and by using an equilibrium transmission amplitude to find the update to the equilibrium T matrix in the presence of a current. As the distribution function entering the right hand side of Eq.(1) does not depend on the spin index m , we find, in linear response, the contribution of the spin flip transmission amplitude Eq.(6) to the off diagonal transmission coefficient $\sum_m \delta T_{mm \Rightarrow ss'}$ for states on the Fermi surface comes from integrating over the Fermi sea

$$\begin{aligned} & f_{ss'}^>(\hat{k}, \varepsilon_F, 0^+) \\ &= \sum_{k,m} \{ t_{ms}^{eq} * \delta t_{ms'}^* + \delta t_{ms} * t_{ms'}^{eq*} \} f^0(\varepsilon_k, 0^-) \\ &= \delta n_z^{int} \sin \theta \{ \Re \overline{t_s V_s^*} [\sigma_{y_r}]_{ss'} + \Im \overline{t_s V_s^*} [\sigma_{x_r}]_{ss'} \}, \quad (11) \end{aligned}$$

where

$$\overline{t_s V_s^*} = \int d\varepsilon_k f^0(\varepsilon_k) g_n(\varepsilon_k) \langle \langle t_s(k_2, k_n; \varepsilon_k) V_s^*(k_s k_n; \varepsilon_k) \rangle \rangle, \quad (12)$$

$t_s(k_2, k_n; \varepsilon_k)$ is the equilibrium transmission amplitude, and the angular brackets are defined in Eq.(9). Here the out of equilibrium densities are $\delta n_z \equiv \frac{1}{2} [\delta n_\uparrow - \delta n_\downarrow]$, and to arrive at this result we made the isotropy assumption for the transmission coefficients so that the angular averages over these coefficients are done independently of those over the distribution function.

This transmission coefficient is current driven so that in linear response it acts on the equilibrium distribution function at the Fermi surface in Eq.(1) to produce an out of equilibrium distribution $f_{ss'}^>$; whereas the transmission Eq.(10) acts on the out of equilibrium distribution

on the Fermi surface. By writing $\delta n_z^{int} \equiv \alpha \delta n_z^l$ and

$$\delta n_z^l = \frac{1}{2} \sum_m [\sigma_{z_l}]_{mm} \int d\Omega_{k'} \delta f_m(\hat{k}'), \quad (13)$$

we find the two contributions, Eqs.(10) and (11), to the T matrix can be written as

$$\begin{aligned} f_{ss'}^>(\hat{k}, \varepsilon_F, 0^+) &= \sum_m T_{mm \Rightarrow ss}(\varepsilon_F) \delta_{ss'} \delta f_m(\hat{k}') + \sum_m \frac{1}{2} \alpha \sin \theta \\ &\times [\sigma_{z_l}]_{mm} \{ \Re \overline{t_s V_s^*} [\sigma_{y_r}]_{ss'} + \Im \overline{t_s V_s^*} [\sigma_{x_r}]_{ss'} \} \delta f_m(\hat{k}'). \quad (14) \end{aligned}$$

Whereas the first term is the equilibrium scattering at the interface in the conventional approach, the second depends on the spin accumulation or current at the interface which is proportional to $\delta f_m(\hat{k}')$, and produces an off diagonal component of the spinor density matrix at the interface. While V_s is a sum over the Fermi surface (see Eq.(9) with $\varepsilon = \varepsilon_F$) and t_s over the entire Fermi sea their difference is made up in the integration over the equilibrium distribution function that enters Eq.(12) which is over Fermi sea. We can only do a meaningful comparison, of the transmission amplitudes in equilibrium and another when one superimposes δn_z^l on the Fermi surface of the normal layer, by calculating the interface scattering for these two situations; interalia this will determine the constant α which indicates how much of the spin accumulation δn_z^l penetrates into the interfacial region so as to affect the interface scattering potential.⁷

By solving the Boltzmann equations of motion we have found that the magnitude of the "out of equilibrium" δT relative to T controls the amount of transverse spin accumulation, but its very existence guarantees the continuity of spin currents at the interface when a steady state is achieved, i.e., to eventually achieve a continuous spin current in the steady state it is necessary that the interface scattering potential has matrix elements that inject transverse spin distributions into a magnetic layer with well defined momentum so that they can propagate past the interface, and into the bulk of a layer.³ Without this additional scattering at the interface we have found a discontinuity in the spin current at all times; while this is found by setting the explicit time derivative of the distribution function, $\partial_t f(k, r, t)$, to zero this solution differs from steady state inasmuch as there is a constant loss of transverse spin current at the interface, i.e., it is questionable whether one can call this a true steady state. The transverse spin current j_y and j_x (this exists if the transmission amplitudes are complex) we calculate in the ferromagnetic layer, by using Eq.(11) or (14), arises from injecting the transverse component of the incoming spin current from a normal layer in such a manner that it excites a transverse mode of propagation in the bulk of the ferromagnetic layer. Our scattering potential provides for the transfer of the transverse spin distribution across an interface in such a manner that it can propagate past the interfacial region and into the bulk of a

magnetic layer; it do not suffer from the dephasing previously found when one considered the transverse spin current that arises from scattering onto different sheets of the Fermi surface, e.g.,

$$T_{mm \Rightarrow ss'} \sim [t_s(k_M)t_{s'}^*(k_m)] \{i/2 \sin \theta \delta_{s'-s}\}, \quad (15)$$

where $k_{M/m}$ represent the Fermi momenta of the majority/minority bands. Among other things the distribution function $f_{ss'}^>(\hat{k}, \varepsilon_F, 0^+)$ found by using this T in Eq.(1) does not have a unique velocity $v(k)$, as $k_M \neq k_m$, therefore it cannot be used to calculate a current within the Boltzmann approach. The existence of this scattering between bands limits transverse currents to a region 1-2 monolayers of the interface,² but it does not negate the current induced interface scattering mechanisms, Eq.(11), that allow for injection into a coherent mode of transverse spin propagation on another length scale.

The spin current transmitted by the conventional coefficients, Eq. (10), is parallel to the local magnetization; it does not have a transverse component. If the interface scattering Eq.(1) is unable to scatter electrons into transverse spin distribution functions $f_{ss'}(k)$ $s' \neq s$ which can propagate past the interfacial region when the current is first turned on, the transverse component of the spin current never leaves the interfacial region; not even in steady state. In a manner of speaking the transverse spin accumulation will remain confined to the interface and one can talk about the spin current as being discontinuous even in the steady state. The two electron scattering across an interface Eq.(3) creates the scattering potential, Eqs.(6) and (11) that allows for a coherent transmission of spin information at the interface. However this only exists at the interface, within a screening length of the interface; without a current this electron distribution does not go beyond the interface scattering

region. In the presence of a current once created at the interface the transverse distribution propagates according to the Boltzmann equation; as the distribution $f_{ss'}$ for $s' \neq s$ does not commute with the Hamiltonian in a magnetic layer (which is described in the spin polarized single electron approximation) we show in another publication this leads to distributions that precess, and that it is the exchange splitting in this approximation $J(k)$ that controls this precession.³ Eventually, this leads to spin accumulation transverse to the magnetization of the magnetic layer, so that in steady state the spin current is continuous across the N/F interface.³

In conclusion our scattering potential provides for the transfer of the transverse spin distribution across an interface in such a manner that it can propagate past the interfacial region and into the bulk of a magnetic layer. The spin flip scattering potential Eq.(6) lies outside the conventional spin polarized single electron treatment of the scattering at a N/F interface as one does not usually envisage when calculating the transmission amplitude a distribution from the spin polarized Fermi surface of a neighboring magnetic layer M_l being superimposed onto the normal layer.⁹ However when one uses an approximate conductivity that is local (short ranged), e.g., when using only the bubble conductivity in the Kubo formalism or the Boltzmann layer by layer approach, in order to account for the long range nature of the conductivity we are required to posit this in the presence of an electric field.^{10,11} The strength of the spin flip potential relative to the ordinary scattering at the interface can be ascertained from calculations of the transmission amplitudes in the presence of spin accumulation in the normal layer.

We would like to thank Arne Brataas, Andrew Kent, Ingrid Mertig, and Shufeng Zhang for very helpful discussions. This work was supported by the National Science Foundation (Grant DMR 0131883).

¹ M.D. Stiles and A. Zangwill, Phys. Rev. B **66**, 014407 (2002). M.D. Stiles and A. Zangwill, J.Appl. Phys. **91**, 6812 (2002).

² J.C. Slonczewski, J. Mag. Mag. Mater. **159**, L1 (1996); *ibid* **195**, L261 (1999); L. Berger, Phys. Rev. B **54**, 9353 (1996); J. Appl. Phys. **89**, 5521 (2001); A. Brataas, Yu.V. Nazarov, and G.E.W. Bauer, Phys. Rev. Lett. **84**, 2481 (2000) and D.H. Hernandez, Y.V. Nazarov, A. Brataas, and G.E.W. Bauer, Phys. Rev.B **62**, 5700 (2000); Alexey Kovalev, Arne Brataas and Gerrit E.W. Bauer, *ibid* **66**, 224424 (2002); M.D. Stiles and A. Zangwill, Phys. Rev. B **66**, 014407 (2002); M.D. Stiles and A. Zangwill, J.Appl. Phys. **91**, 6812 (2002); J.C. Slonczewski, J. Mag. Mag. Mater. **247**, 324 (2002); Gerrit.E.W. Bauer, Yaroslav Tserkovnyak, Daniel Huertas-Hernando and Arne Brataas, Phys. Rev. B **67**, 094421 (2003).

³ Jianwei Zhang, Peter M. Levy, Shufeng Zhang and Vladimir Antropov, submitted for publication.

⁴ X. Waintal, E.B. Myers, P.W. Brouwer and D.C.

Ralph, Phys. Rev.B **62**, 12 317 (2000); Gerrit E.W. Bauer, Yaroslav Tserkovnyak, Daniel Huertas-Hernando and Arne Brataas, Adv. in Solid State Physics, **43**, 383 (2003). Note only states accessible in equilibrium (see Eqs.(10) and (15)) are considered in these references.

⁵ Coherences in the distribution function are the off diagonal elements of statistical density matrix; here we are interested in those induced by currents across noncollinear magnetic structures at the Fermi surface.

⁶ A. Messiah, **Quantum Mechanics, Vol.II**, (North-Holland, Amsterdam, John Wiley, New York, 1961-62); see Chap.XIX, Secs. 11-13.

⁷ A realistic evaluation of the transmission coefficient Eq.(14) is being undertaken by using spin polarized single electron states for a Cu/Co interface; I. Mertig , private communication.

⁸ In the situation envisaged in Figs. 3c and 3d of M.D. Stiles and A. Zangwill, J.Appl. Phys. **91**, 6812 (2002) we see that the transverse components of the spin fluxes are annih-

lated on opposite sides of the normal spacer layer between two noncollinear magnetic layers.

⁹ The possibility for spin flip scattering at interfaces was envisaged in the papers of Bauer's group, see Refs.2 and 4, but their origin was not discussed nor was their role included in the analyses.

¹⁰ P.M. Levy, H.E. Camblong and S. Zhang, J. Appl. Phys. **75**, 7076 (1994); H.E. Camblong, P.M. Levy and S. Zhang, Phys. Rev. B **51**, 16052 (1995).

¹¹ C.L. Kane, R.A. Serota and P.A. Lee, Phys. Rev. B **37**, 6701 (1988).